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     (FILE 'HOME' ENTERED AT 15:27:02 ON 11 MAR 2008)

     FILE 'USPATFULL, WPIDS' ENTERED AT 15:27:26 ON 11 MAR 2008
L1          109 FILE USPATFULL
L2            5 FILE WPIDS
     TOTAL FOR ALL FILES
L3          114 S (QUANTUM MECHANICS) AND (MOLECULAR MECHANICS) AND SIMULAT?
L4           85 FILE USPATFULL
L5            2 FILE WPIDS
     TOTAL FOR ALL FILES
L6           87 S (QUANTUM MECHANICS) AND (MOLECULAR MECHANICS) AND SIMULAT? AN

     FILE 'USPATFULL' ENTERED AT 15:44:01 ON 11 MAR 2008
L7           63 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L8            0 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L9            0 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L10           0 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L11           0 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L12          86 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L13          48 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) (P) SIMULAT?

=> d l13 5,12,13 bib,kwic

L13  ANSWER 5 OF 48  USPATFULL on STN
AN     2007:49718  USPATFULL
TI     Molecular simulation method and device
IN     Yonezawa, Yasushige, Suita-shi, JAPAN
       Takada, Toshikazu, Minato-ku, JAPAN
       Nakata, Kazuto, Minato-ku, JAPAN
       Sakuma, Toshihiro, Minato-ku, JAPAN
       Nakamura, Haruki, Suita-shi, JAPAN
PA     NEC CORPORATION, Tokyo, JAPAN (non-U.S. corporation)
       OSAKA UNIVERSITY, Osaka, JAPAN (non-U.S. corporation)
PI     US 2007043545       A1  20070222
AI     US 2004-573023      A1  20040922 (10)
       WO 2004-JP13808         20040922
                               20060322  PCT 371 date
PRAI   JP 2003-329751      20030922
DT     Utility
FS     APPLICATION
LREP   DICKSTEIN SHAPIRO LLP, 1177 AVENUE OF THE AMERICAS (6TH AVENUE), NEW
       YORK, NY, 10036-2714, US
CLMN   Number of Claims: 18
ECL    Exemplary Claim: 1
DRWN   3 Drawing Page(s)
LN.CNT 754
SUMM    The present invention relates to a method and a device for performing
       molecular simulation by a quantum chemical technique, and more
       particularly relates to a molecular simulation method and a
       device by a QM/MM (Quantum Mechanics/
       Molecular Mechanics) method in which the ab initio
       molecular orbital method and the molecular mechanics
       method are combined as one theoretical system among theoretical
       techniques of the quantum chemistry.
SUMM    . . . the like are limited. Therefore, it is considered that only
       the sites and the vicinity thereof are subjected to accurate
       simulation about electron states. Accordingly, in a chemical
       system including many molecules, the QM/MM method is proposed in which a
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molecule or a part of molecule is divided into a QM (Quantum Mechanics) space where a noted chemical phenomenon occurs and a secondary MM (Molecular Mechanics) space other than the QM space and in which the QM space is processed by a quantum mechanical scheme such as the ab initio molecular orbital method and the MM space is described as empirical potential such as molecular mechanics [1]. Advantages of this method are following:

L13 ANSWER 12 OF 48 USPATFULL on STN
AN 2005:319379 USPATFULL
TI Methods for molecular property modeling using virtual data
IN Duffy, Nigel P., San Francisco, CA, UNITED STATES
Lanza, Guido, San Francisco, CA, UNITED STATES
Yu, Jessen, San Francisco, CA, UNITED STATES
Mydlowec, William, San Francisco, CA, UNITED STATES
PI US 2005278124 A1 20051215
AI US 2005-74587 A1 20050308 (11)
PRAI US 2004-579619P 20040614 (60)
DT Utility
FS APPLICATION
LREP RAYMOND R. MOSER JR., ESQ., MOSER IP LAW GROUP, 1040 BROAD STREET, 2ND FLOOR, SHREWSBURY, NJ, 07702, US
CLMN Number of Claims: 39
ECL Exemplary Claim: 1
DRWN 4 Drawing Page(s)
LN.CNT 808
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
DETD . . . included in the training data may be provided using "virtual data," and may include information obtained from reasonable assumptions, computer simulations, or other modeling efforts. For example, computer simulations may be performed that simulate the physics of the molecular property of interest using molecular mechanics or quantum mechanics. Property information may also be obtained from laboratory experimentation or published literature sources. Additionally, property information may include a measure. . .

L13 ANSWER 13 OF 48 USPATFULL on STN
AN 2005:196237 USPATFULL
TI Lead molecule cross-reaction prediction and optimization system
IN Kita, David, Milpitas, CA, UNITED STATES
Fodor, Eniko, Fremont, CA, UNITED STATES
Prakash, Adityo, Fremont, CA, UNITED STATES
PA Verseon, Milpitas, CA, UNITED STATES (U.S. corporation)
PI US 2005170379 A1 20050804
AI US 2004-966341 A1 20041014 (10)
PRAI US 2003-511474P 20031014 (60)
DT Utility
FS APPLICATION
LREP TOWNSEND AND TOWNSEND AND CREW, LLP, TWO EMBARCADERO CENTER, EIGHTH FLOOR, SAN FRANCISCO, CA, 94111-3834, US
CLMN Number of Claims: 70
ECL Exemplary Claim: 1
DRWN 25 Drawing Page(s)
LN.CNT 3120
DETD . . . earlier in both the background section and the detailed technical description, including standard shape complementarity methods, conventional techniques based on molecular mechanics paradigms, molecular dynamics and/or quantum mechanics simulations, QSAR, free energy perturbation theory, or even the utilization of various empirically derived or knowledge-based scoring

function.

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L12          86 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) AND SIMULAT?
L13          48 S (((QUANTUM MECHANICS) (P) (MOLECULAR MECHANICS)) (P) SIMULAT?

=> d l2 1-5 bib,kwic
YOU HAVE REQUESTED DATA FROM FILE 'WPIDS' - CONTINUE? (Y)/N:y
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L2 ANSWER 1 OF 5 WPIDS COPYRIGHT 2008 THE THOMSON CORP on STN
AN 2008-A36197 [03] WPIDS
DNN N2008-028101 [03]
TI Method of positioning polyphenols compound antioxidant point
DC S03; T01
IN LV L
PA (UYNA-N) UNIV NANJING
CYC 1
PIA CN 101000354 A 20070718 (200803)* ZH [1]
ADT CN 101000354 A CN 2006-10166311 20061226
PRAI CN 2006-10166311 20061226
NOV NOVELTY - The invention claims a method of positioning polyphenols compound antioxidant point. specifically the MM + molecular mechanics method of testing polyphenols compound is used for processing primary optimizing structure calculation, then the semi-empirical AM1 quantum mechanics method is used for processing further optimizing calculation, finally Gaussian 03 program with abinitio calculation HF method is used for.. . . as the amount of the net electronic charge of dissociation energy and atom, then the hyperoxidation revulsant is used for simulating oxidation reaction, the segregative oxidation metabolite is identified its structure, after that it assures the active point after oxidation reaction.. . . only makes up the deficiency under the ideal condition calculating, but also avoids the inferential deviation of complex metabolite by simulating oxidation reaction, and it is able to test the polyphenols compound antioxidant point.

L2 ANSWER 2 OF 5 WPIDS COPYRIGHT 2008 THE THOMSON CORP on STN
AN 2005-285012 [29] WPIDS

DNC C2005-088424 [29]
DNN N2005-233808 [29]
TI   Molecular simulation in chemical industry, involves dividing
     molecule into quantum mechanics space and
     molecular mechanics space and applying non-empirical
     molecule orbital method to quantum mechanics space
DC   J04; T01
IN   NAKAMURA H; NAKATA K; SAKUMA T; TAKADA T; YONEZAWA Y
PA   (NIDE-C) NEC CORP; (OSAU-C) UNIV OSAKA
CYC 106
PIA WO 2005029385   A1 20050331 (200529)* JA 28[5]
     JP 2005514101   X 20061130 (200681) JA 18
     US 20070043545 A1 20070222 (200717) EN
ADT WO 2005029385 A1 WO 2004-JP13808 20040922; JP 2005514101 X WO 2004-JP13808
     20040922; JP 2005514101 X JP 2005-514101 20040922; US 20070043545 A1 WO
     2004-JP13808 20040922; US 20070043545 A1 US 2006-573023 20060322
FDT JP 2005514101   X Based on WO 2005029385   A
PRAI JP 2003-329751   20030922
TI   Molecular simulation in chemical industry, involves dividing
     molecule into quantum mechanics space and
     molecular mechanics space and applying non-empirical
     molecule orbital method to quantum mechanics space
TT   TT: MOLECULAR SIMULATE CHEMICAL INDUSTRIAL DIVIDE QUANTUM
         MECHANICAL SPACE APPLY NON EMPIRICAL ORBIT METHOD
NOV NOVELTY - A molecule to be simulated is divided into
     quantum mechanics (QM) space and molecular
     mechanics (MM) space. A non-empirical molecule orbital method is
     applied to the QM space with an empirical potential.
DETD DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the
     following:
          (1) a molecular simulation apparatus;
          (2) a molecular simulation program; and
          (3) recording media storing molecular simulation program.
USE
     USE - Used for performing molecular simulation of a living
     organism in the chemical industry, and during the manufacture of
     pharmaceutical and functional food, and also in. . .
ADV ADVANTAGE - The molecular simulation is performed with high
     reliability.
DRWD DESCRIPTION OF DRAWINGS - The figure shows a flowchart illustrating
     molecular simulation. (Drawing includes non-English language
     text).

L2   ANSWER 3 OF 5 WPIDS COPYRIGHT 2008   THE THOMSON CORP on STN
AN   2004-088951 [09]   WPIDS
DNC C2004-036271 [09]
DNN N2004-071198 [09]
TI   Development of molecular mechanics force field
     parameters involves exporting the optimized force field parameters to
     external molecular mechanics simulation
     packages and saving optimize force field parameters to the database
DC   B04; J04; T01
IN   SUN H
PA   (SUNH-I) SUN H
CYC 1
PIA US 20030195734 A1 20031016 (200409)* EN 17[3]
     US 6785665   B2 20040831 (200457) EN
ADT US 20030195734 A1 US 2002-139806 20020416
PRAI US 2002-139806   20020416
TI   Development of molecular mechanics force field
     parameters involves exporting the optimized force field parameters to

external molecular mechanics simulation
packages and saving optimize force field parameters to the database
TT TT: DEVELOP MOLECULAR MECHANICAL FORCE FIELD PARAMETER OPTIMUM EXTERNAL SIMULATE PACKAGE SAVE DATABASE
NOV NOVELTY - Molecular mechanics force field parameters
are developed by importing molecular models representing the molecular systems to be parameterized, validating the estimated and optimized force field parameters, and exporting the optimized force field parameters in required formats to external molecular mechanics
simulation packages and saving the molecular models, input data
and optimize force field parameters to the database.
DETD DETAILED DESCRIPTION - Development of molecular
mechanics force field parameters comprises creating or importing
molecular models that represent the molecular systems to be parameterized, searching a database. . . the molecular models and stored molecular models and retrieving stored parameters if complete matches are found, preparing input data for quantum mechanics ab initio
calculations for the molecular models, importing calculated data of the quantum mechanics ab initio calculations for the
molecular models, selecting force field type and functional forms, and assigning atom types to the. . . set of mathematical formulas for the molecular models, optimizing the initial force field parameters to fit the input data of quantum mechanics ab initio
calculations, validating the optimized force field parameters, and exporting the optimized force field parameters in required formats to external molecular mechanics simulation
packages and saving the molecular models, input data and optimize force field parameters to the database.
USE
USE - For developing molecular mechanics force field
parameters for computer simulations of molecular systems, which include molecules, clusters of molecules and clusters of atoms.
ADV ADVANTAGE - The inventive method is capable of rapidly and easily provides high quality molecular mechanics force fields that are
required for successful computer modeling in chemical, pharmaceutical and material industries

L2 ANSWER 4 OF 5 WPIDS COPYRIGHT 2008 THE THOMSON CORP on STN
AN 1999-418399 [35] WPIDS
DNC C1999-122896 [35]
DNN N1999-312326 [35]
TI Calculating relative stabilities of two molecules from conformational free energies
DC A35; B02; B04; D15; D16; E37; T01
IN KOLOSSVARY I
PA (UYCO-C) UNIV COLUMBIA NEW YORK
CYC 23
PIA WO 9917222 A1 19990408 (199935)* EN 88[4]
AU 9897796 A 19990423 (199935) EN
US 6178384 B1 20010123 (200107) EN
ADT WO 9917222 A1 WO 1998-US20368 19980929; US 6178384 B1 US 1997-940145 19970929; AU 9897796 A AU 1998-97796 19980920
FDT AU 9897796 A Based on WO 9917222 A
PRAI US 1997-940145 19970929
ADV. . . method should identify agents with greater specificity for, and activity at, target sites. It does not require expensive free energy simulations or computational 'alchemy'.
TECH. . . .
The low-energy minimum conformations are 15-35 kJ/mole above the lowest energy conformation and the potential energy function is based on molecular mechanics or on ab initio, semi-empirical or

density-functional quantum mechanics. The atomic co-ordinates used are external (Cartesian) or internal (bond lengths, bond or torsional angles) and Hi is exact or.. . .

Member(0003)
ABEQ US 6178384 . . .
method should identify agents with greater specificity for, and activity at, target sites. It does not require expensive free energy simulations or computational 'alchemy'.

L2 ANSWER 5 OF 5 WPIDS COPYRIGHT 2008 THE THOMSON CORP on STN
AN 1996-363502 [37] WPIDS
DNC C1996-114569 [37]
DNN N1996-306432 [37]
TI Construction of molecular models, e.g. for drug design - providing accurate 3-dimensional geometry by successive addition of fragments which regard the binding site region in a special way
DC B04; J04; S05; T01
IN FERINCZ J; KRIEG B
PA (FERI-I) FERINCZ J; (KRIE-I) KRIEG B
CYC 1
PIA DE 19504724 A1 19960808 (199637)* DE 10[6]
ADT DE 19504724 A1 DE 1995-19504724 19950201
PRAI DE 1995-19504724 19950201
USE USE - The system is based on a numerical process (molecular mechanics, quantum mechanics, or molecular dynamics) or an expert system. It is useful for determining the 3-dimensional geometry of molecules in organic chemistry, biochemistry, molecular biology and related sciences, e.g. in understanding reaction mechanisms, developing and improving drugs (`drug design') and simulating chemical reactions using computers.